Chemistry 7940
Quantum Mechanics II
Spring 2013

Course topics

LAST REVISED: January 15, 2013

1. Density matrix
   - Pure vs mixed states. Ensemble interpretation.
   - Reduced density matrices.
   - Correlation & entanglement. Bell’s theorem.
   - Equations of motion. Analogy with classical mechanics.
   - Relaxation and decoherence.
   - Generalized measurements, quantum information theory, and all that.

2. Time-dependent phenomena
   - Evolution operator. Propagators and Green’s functions.
   - Three pictures: Schrödinger, Heisenberg, interaction.
   - Sudden approximation.
   - Adiabatic approximation. Geometric phases.
   - Perturbation theory for the density operator. Linear response.

3. Path integral formulation of quantum mechanics (brief)
   - Derivation of the sum-over-paths expression for the propagator.
   - Semiclassical limit of the path integral.
   - Path integral formulation of quantum statistical mechanics: polymer beads, and all that.

4. Molecule-field interactions
   - Brief review: Maxwell’s equations, scalar and vector potentials, gauge transformations, free field, and all that.
   - Derivation of Hamiltonian for charged particle in field.
   - Perturbation in dipole approximation.
   - Electric quadrupole and magnetic dipole transitions.
   - High-order perturbation theory and multiphoton processes.
   - Nonlinear spectroscopy.
   - Electric and magnetic properties of molecules (brief).
   - Quantizing the EM field. Photons. Spontaneous emission revisited.
5. Quantum mechanics of the continuum: Scattering theory
   - Particle flux and scattering cross sections.
   - Green’s functions and the scattering problem.
   - Born approximation.
   - Partial wave analysis of wavefunction for central scattering potential.
   - Phase shifts and the differential cross section.

If we have time:

6. Group theory in quantum mechanics
   - Fundamentals (briefly): groups; classes; cosets; representations; irreps; Schur’s lemma.
   - Great Orthogonality Theorem.
   - Characters; character tables.
   - Representation theory and QM. Symmetry and degeneracy.
   - Projection operators.
   - Rotation group: spherical tensors; Wigner-Eckart theorem.

7. Introduction to molecular spectroscopy
   - Born-Oppenheimer approximation.
   - Rotation-vibration separability.
   - Normal modes.